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Phenyl 2-oxoimidazolidine-1-carboxylate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.064
wR factor = 0.131
Data-to-parameter ratio = 12.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_{10}H_{10}N_2O_3$, the five-membered imidazolidine ring is planar, with an r.m.s. derivation of 0.0243 (1)Å. The dihedral angle between the imidazolidine ring and the phenyl ring is 78.83 (2)°. A centrosymmetric ring is formed by a pair of N—H···O hydrogen bonds, creating a dimer; C—H···O hydrogen bonds connect these dimers into a three-dimensional network.

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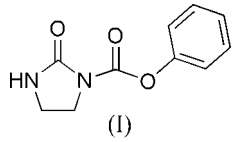
Comment

Imidazolidine derivatives have become important intermediates and building blocks in the construction of various biologically active compounds (Wang *et al.*, 1995; Anderson *et al.*, 1982). A number of methods have been described in the literature for the prepartion of these compounds (Coldham *et al.*, 1998; Katritzky *et al.*, 2002). A simple, efficient and practical procedure for imidazolidines has also been reported by members of our laboratory (Su *et al.*, 2000).



(I)

In the title compound (I) (Fig. 1), the five-membered imidazolidine ring is planar with an r.m.s. derivation of 0.0243 (1) Å. The dihedral angle between the imidazolidine and phenyl rings is 78.83 (2)°.

The crystal packing of (I) is dominated by hydrogen bonds (Table 1). The N2—H2···O3^{i} hydrogen bond creates a molecular dimer; these dimers are connected by C—H···O hydrogen bonds into a three-dimensional network (Fig. 2). The crystal packing is also reinforced by a C10—H10*A*···π interaction with the (C1^{i}—C6^{i}) ring of 3.558 (2) Å [symmetry code: (i) $-x, \frac{1}{2}+y, \frac{1}{2}-z$].

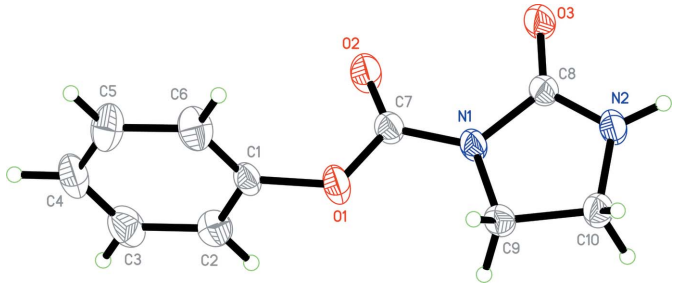


Figure 1
The molecular structure of (I) with the atom numbering and displacement ellipsoids drawn at the 50% probability level.

Experimental

A mixture of phenol (12 mmol), 10% aqueous sodium hydroxide (4 ml), crushed ice (400 mmol) and 2-oxoimidazolidine-1-carbonyl chloride (10 mmol) was stirred for 2 h to give the title compound in 81% yield. Single crystals suitable for data collection were obtained by slow evaporation of an ethanol solution (457–458 K).

Crystal data

$C_{10}H_{10}N_2O_3$
M_r = 206.20
Monoclinic, $P2_1/c$
a = 6.3535 (8) Å
b = 14.0240 (18) Å
c = 10.8840 (13) Å
β = 95.207 (3)°
V = 965.8 (2) Å^3
Z = 4
D_x = 1.418 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 (2) K
Block, colourless
0.15 × 0.12 × 0.07 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.984, T_{max} = 0.993
4994 measured reflections
1704 independent reflections
1156 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.131
S = 1.07
1704 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2 + 0.232P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3^{i}	0.86	2.04	2.872 (3)	161
C4—H4···O3^{ii}	0.93	2.62	3.218 (4)	123
C2—H2A···O3^{iii}	0.93	2.48	3.403 (4)	175
C10—H10B···O2^{iv}	0.97	2.83	3.690 (4)	148

Symmetry codes: (i) $-x-1, -y+1, -z$; (ii) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $x+1, y, z$; (iv) $-x, -y+1, -z$.

The H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of Csp^2—H = 0.93 and N—H = 0.86 Å, with U_{iso} = 1.2U_{eq}(C,N) and Csp^3—H = 0.97 Å with U_{iso} = 1.5U_{eq}(C).

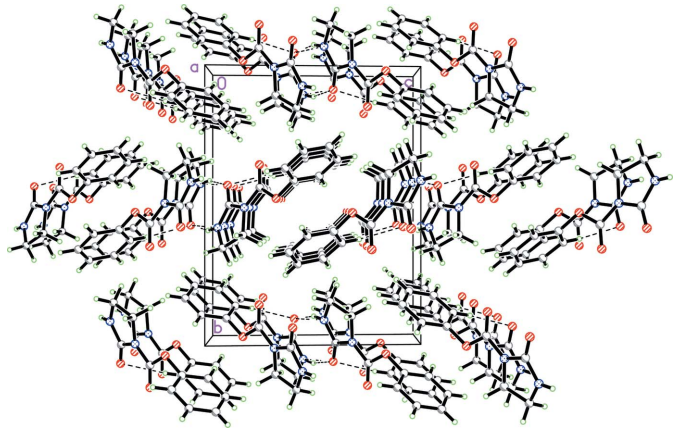


Figure 2
The packing of (I) showing the three-dimensional network formed by hydrogen bonds (shown as dashed lines).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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